

ABSTRACT

The present invention is directed to serve ligand screening apparatuses, ligand screening methods, programs and a recording medium for studying the binding analysis between a receptor including an induced-fit type receptor and a ligand. First, analysis and calculation of normal mode are conducted, and then fluctuation of a dihedral angle of a main chain in a steady state is calculated. Then by carrying out a molecular dynamic calculation while imposing constraint on each atom based on the fluctuation, a dynamic structure of the receptor is predicted more accurately. By using the dynamic structure obtained in the molecular dynamic calculation and an interaction function, receptor/ligand binding which is also applicable to an induced-fit type receptor is predicted with high accuracy.